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The Interplay of manganese and nitrate in hydroxyapatite nanoparticles as revealed by pulsed EPR and DFT

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Abstract

© the Owner Societies 2015. The interplay of oppositely charged substitutions in the structure of hydroxyapatite (HAp) nanopowders is investigated on the atomic level by pulsed electron paramagnetic resonance (EPR) technique and ab initio density functional theory calculations. Benefits of EPR to determine Mn^{2+} ions in nano-HAp samples are demonstrated. A simple approach based on the measurements of electron spin relaxation times allowed observing the strong influence of fast-relaxing Mn^{2+} ions on the relaxation characteristics of the nitrate ions ($NO3^{-}$/$NO3^{2-}$) incorporated in trace amounts. Based on the results of ab initio calculations, we show the propensity of Mn^{2+} and $NO3^{-}$/$NO3^{2-}$ to associate within the HAp crystal lattice. This could have a direct impact on the functional properties of the material especially to resorption and ion exchange. Furthermore, such an effect can increase a propensity of undesired impurities to incorporate into the doped nanocrystals.

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